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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
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EXAMINER

NEGIN, RUSSELL SCOTT

ART UNIT	PAPER NUMBER
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1631

NOTIFICATION DATE	DELIVERY MODE
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10/30/2008

ELECTRONIC

Please find below and/or attached an Office communication concerning this application or proceeding.

The time period for reply, if any, is set in the attached communication.

Notice of the Office communication was sent electronically on above-indicated "Notification Date" to the following e-mail address(es):

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Office Action Summary	Application No. 10/723,594	Applicant(s) PANG, YUAN-PING	
	Examiner RUSSELL S. NEGIN	Art Unit 1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☐ Responsive to communication(s) filed on 10 July 2008.
- 2a) ☐ This action is **FINAL**. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 37-72 is/are pending in the application.
- 4a) Of the above claim(s) _____ is/are withdrawn from consideration.
- 5) ☐ Claim(s) _____ is/are allowed.
- 6) ☒ Claim(s) 37-72 is/are rejected.
- 7) ☐ Claim(s) _____ is/are objected to.
- 8) ☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☒ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on _____ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some * c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
 2. ☐ Certified copies of the priority documents have been received in Application No. _____.
 3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- | | |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892) | 4) <input type="checkbox"/> Interview Summary (PTO-413) |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | Paper No(s)/Mail Date. _____ |
| 3) <input checked="" type="checkbox"/> Information Disclosure Statement(s) (PTO/SB/08) | 5) <input type="checkbox"/> Notice of Informal Patent Application |
| Paper No(s)/Mail Date <u>7/10/2008</u> . | 6) <input type="checkbox"/> Other: _____ |

DETAILED ACTION

Comments

Applicants' amendments and request for reconsideration in the communication filed on 10 July 2008 are acknowledged and the amendments are entered.

Claims 37-72 are pending and examined in the instant application.

Withdrawn Rejections

The rejections of claims 37-72 under 35 U.S.C. 112, first paragraph are withdrawn in view of arguments on page 7-9 of the Remarks of 10 July 2008.

Information disclosure statement

The information disclosure statement filed on 10 July 2008 has been considered.

Priority

While the instant application claims benefit to application 09/595,650 filed on 16 June 2000 and provisional application 60/139,845 filed on 18 June 1999, the provisional application only discloses the relevant method, and NOT the "machine having a processor and data storage medium" as recited in claim 37 OR the "computer readable data storage medium having computer executable instructions stored thereon" as recited in instant claim 55.

Additionally, application 09/595,650, as originally filed (and now abandoned) only discloses the relevant method, and NOT the "machine having a processor and data

storage medium” as recited in claim 37 OR the “computer readable data storage medium having computer executable instructions stored thereon” as recited in instant claim 55. Since all of the instantly pending claims depend from instant claim 37 or 55, all of the instant claims receive benefit only to the divisional application filed on 26 November 2003 and not to the provisional application filed on 18 June 1999.

Specification

The following objection is newly applied:

The amendment filed 9 April 2004 is objected to under 35 U.S.C. 132(a) because it introduces new matter into the disclosure. 35 U.S.C. 132(a) states that no amendment shall introduce new matter into the disclosure of the invention. The added material which is not supported by the original disclosure is as follows: the "machine having a processor" as recited in claim 37 AND the “computer readable data storage medium having computer executable instructions stored thereon” as recited in instant claim 55. These limitations are not disclosed in the original disclosures of the instant application or the parent applications.

Applicant is required to cancel the new matter in the reply to this Office Action.

Claim Rejections - 35 USC § 112

The following is a quotation of the first paragraph of 35 U.S.C. 112:

The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and use the same and shall set forth the best mode contemplated by the inventor of carrying out his invention.

The following rejection is newly applied:

Claims 37-72 are rejected under 35 U.S.C. 112, first paragraph, as failing to comply with the written description requirement. The claim(s) contains subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the relevant art that the inventor(s), at the time the application was filed, had possession of the claimed invention. The "machine having a processor and data storage medium" as recited in claim 37 AND the "computer readable data storage medium having computer executable instructions stored thereon" as recited in instant claim 55 are not disclosed in the original disclosures of the instant application or the parent applications.

Claim Rejections - 35 USC § 101

The following rejection is reiterated from the previous Office action and is newly applied for claims 37-54:

35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

Claims 37-72 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

Claim 37 is drawn to a machine having a processor and a data storage medium. Since the specification is silent on what constitutes "data storage medium," this claim can be interpreted broadly such that this "data storage medium" encompasses, for example, intangible media such as carrier waves which, per se, are not statutory.

Consequently, an embodiment of claims 37-54 results in a set of claims that is not statutory. See MPEP 2106.

Claim 55 is drawn to a computer readable medium having computer executable instructions stored thereon to execute a simulation. Since the specification is silent on what constitutes "computer readable media," this claim can be interpreted broadly such that this "computer readable media" encompasses in tangible media such as carrier waves which, per se, are not statutory. Consequently, an embodiment of claims 55-72 results in a set of claims that is not statutory. See MPEP 2106.

Response to Arguments:

Applicant's arguments filed 7 December 2007 have been fully considered but they are not persuasive.

Applicant argues that the media recited in the instant claims are not interpretable to encompass carrier waves. This is not persuasive because there are other intangible forms of data storage media and computer readable media that do NOT encompass carrier waves; carrier waves merely exemplify this phenomenon.

Claim Rejections - 35 USC § 103

The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

The following rejection is newly applied:

35 U.S.C. 103 Rejection #1:

Claims 37-47, 52-65, and 70-72 are rejected under 35 U.S.C. 103(a) as being unpatentable over Andriotis et al. [Chemical Physics Letters, 5 March 1999, volume 301, pages 503-508] in view of Stote et al. [Proteins: Structure, Function, and Genetics; 1995, volume 23, pages 12-31].

Claim 37 is drawn to a machine having a processor and a data storage medium, the processor communicatively coupled to the data storage medium, and the data storage medium storing instructions for performing a method comprising:

- receiving information relating to a monoatomic metal ion to be simulated;
- and generating, for observation by a user on a display, a representation of the monoatomic metal ion as a metal molecule by a molecular dynamics simulation, wherein said metal molecule comprises a plurality of atoms comprising a center atom and one or more dummy atoms, wherein said center atom has a van der Waals radius greater than zero, wherein said center atom is covalently linked to said one or more dummy atoms, and wherein each dummy atom has a positive charge.

Claim 55 is drawn to a computer readable data storage medium having computer executable instructions stored thereon to perform the method executed by the machine in instant claim 37.

The article of Andriotis et al. is a tight-binding molecular dynamics study of transition metal carbide clusters.

Specifically, Andriotis et al. simulates nickel-carbide clusters such that the monoatomic metal ion to be simulated is nickel. Figure 1-3 of Andriotis et al. illustrate as a display, a representation of the monoatomic ion that is simulated as metal molecules. The center atom is neutral carbon (has a radius greater than zero) and the dummy atoms are the nickels (positively charged with a radius of about zero). The carbon is covalently linked to at least one nickel. It is noted that the claims do not limit the center atom to be a metal atom, thus the claims are reasonably and broadly interpreted where the metal molecule comprises a central atom other than a metal as well as those where both the central atom and dummy atoms are metal atoms.

Andriotis et al. does not show a machine having a processor and a data storage medium wherein the processor is communicatively coupled to the data storage medium.

The article of Stote et al. studies zinc binding to proteins and solution. The acknowledgements section on page 29 of Stote et al. teaches use of CRAY, SGI, and SUN workstations to process the molecular dynamics simulations of zinc binding to proteins.

With regards to claims 38-39 and 56-57, the dummy atom nickel in Andriotis et al. has a mass of about or greater than about 0.1 g/mol.

With regard to claims 40-43 and 58-61, polyhedrons are illustrated in Figure 1-3 of Andriotis et al. wherein the dummy atoms of nickel are at the apices and the center

Art Unit: 1631

atom carbon is in the center of the polyhedron. Figure 1 of Andriotis et al. also illustrates a tetrahedron.

With regards to claims 44-45 and 62-63, the metal ion is the transition metal nickel in Figures 1-3 of Andriotis et al.

With regard to claims 46-47 and 64-65, Stote et al. simulates zinc (see title and abstract).

With regard to claims 52-54 and 70-72, the nickel in Andriotis et al. has a charge of about +.5, +.3333, and between about 0.1 and about +3 (i.e. see Table 1 of Andriotis et al.)

It would have been obvious to someone of ordinary skill in the art at the time of the instant invention to modify the simulation of nickel-carbide clusters of Andriotis et al. by use of the modeling of a metal using advanced computer systems as taught by Stote et al. wherein the motivation would have been that the computer apparatus of Stote et al. have the advantage of fast, and accurate simulation [i.e. see Acknowledgements on page 29 of Stote et al.] It would have been further obvious to substitute zinc in Stote for the nickel in Andriotis et al. to yield the predictable result of an alternate method of simulating carbide complexes. There would have been a reasonable expectation of

Art Unit: 1631

success in substituting zinc for nickel because they are both transition elements with analogous properties in *in silico* molecular dynamics simulations.

The following rejection is newly applied:

35 U.S.C. 103 Rejection #2:

Claims 48-51 and 66-69 are rejected under 35 U.S.C. 103(a) as being unpatentable over Andriotis et al. in view of Stote et al. as applied to claims 37-47, 52-65, and 70-72 above, and further in view of Aqvist et al. [Journal of the American Chemical Society, 1990, volume 112, pages 2860-2868; on IDS].

Claims 48 and 66 further limit the metal to be magnesium.

Claims 49 and 67 further limit the metal to be calcium.

Claims 50 and 68 are further limiting wherein the metal has a calculated energy of solvation about equal to an experimentally determined energy of solvation for the metal.

Claims 51 and 69 are further limiting wherein the calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.

Andriotis et al. and Stote et al. make obvious a computerized method for simulating metal ions, as discussed above.

Andriotis et al. and Stote et al. do not simulate magnesium and calcium. Additionally, Andriotis et al. and Stote et al. do not find energies of solvation.

Aqvist et al. studies free energy relationships in metalloenzyme-catalyzed reactions.

Specifically, Figure 3 of Aquist et al. compares calculated energies of solvation of calcium and magnesium with observed values.

It would have been obvious to someone of ordinary skill in the art at the time of the instant invention to modify the zinc and nickel metal ion simulation methods of Andriotis et al. and Stote et al. by use of the calcium and magnesium in Aquist et al. because it is obvious to substitute known elements in the prior art to yield a predictable result. In this instance, calcium and magnesium are alternate metal ions for simulation as nickel and zinc. There would have been a reasonable expectation of success in combining Andriotis et al., Stote et al. and Aquist et al. because all of the ions discussed are metals with analogous properties in *in silico* molecular dynamics simulations. It would have been further obvious to apply the simulated energies of solvation of Aquist et al. to the simulations of Andriotis et al. and Stote et al. because Aquist et al. presents calculated energetics in agreement with experimental data (i.e. see Figure 3 of Aquist et al.).

Response to Arguments

Applicant's additional arguments with respect to claims 37-72 have been considered but are moot in view of the new ground(s) of rejection.

Conclusion

Art Unit: 1631

No claim is allowed.

Papers related to this application may be submitted to Technical Center 1600 by facsimile transmission. Papers should be faxed to Technical Center 1600 via the central PTO Fax Center. The faxing of such pages must conform with the notices published in the Official Gazette, 1096 OG 30 (November 15, 1988), 1156 OG 61 (November 16, 1993), and 1157 OG 94 (December 28, 1993)(See 37 CFR § 1.6(d)). The Central PTO Fax Center Number is (571) 273-8300.

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Russell Negin, Ph.D., whose telephone number is (571) 272-1083. The examiner can normally be reached on Monday-Friday from 7am to 4pm.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's Supervisor, Marjorie Moran, Supervisory Patent Examiner, can be reached at (571) 272-0720.

Information regarding the status of the application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information on the PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

/RSN/
Russell S. Negin, Ph.D.
21 October 2008

/Marjorie Moran/
Supervisory Patent Examiner, Art Unit 1631